



**June 25-28, 2013**

**Advances in Photoreactions: When spin-orbit coupling, optical excitation, and nuclei motion are of equal importance?**

**The workshop targets synergy of experimental and computational descriptions of excited electronic state and reaction dynamics in a broad range of nano-structured materials for luminescent, photovoltaic, and photocatalytic applications.** Theoretical advances are needed for interpretation of experimental data and applications ranging from spectroscopy of color centers in laser crystals, transition metal ions and lanthanide ions in solid host matrices and coordination complexes, to charge transfer in semiconductor nanocrystals for photovoltaics and surface reactions for photocatalysis, as well as molecular magnets, and biological labels.

This workshop presents current frontiers in computational and experimental studies of basic photo-induced processes: light absorption, luminescence, hot carrier relaxation, formation and breaking of charge transfer excitations, and reaction dynamics at catalytic sites with heavy elements – all perturbed by environment such as lattice vibrations and solvent polarization and, therefore, have to be treated with "open system" approach.

Open challenges arise in interpreting processes with spin-orbit coupling, optical excitation and motion of nuclei. Non-adiabatic dynamics, on-the-fly coupling, surface hopping, and density matrix equation of motion became computational tools of choice for ab initio treatment of non-equilibrium dynamics in molecules and nanostructures.

**Invited Speakers:**

Rich Martin (Los Alamos)  
Daniel Gargas (LBL)  
Kenneth Lopata (PNNL)  
Jacek Jakowski (Oakridge)

Mary Berry (USD)  
Toru Shiozaki (Northwestern)  
Artem Masunov (UCF)  
Benjamin Levine (MSU)

P. Stanley May (USD)  
Spiridoula Matsika (Temple U.)  
Kirill Velizhanin (LANL)  
Elena Jakubikova (North Carolina SU)

**International Advisory Committee:**

Rich Martin (Los Alamos)  
Mike Reed (Cantebury, New Zealand)  
Todd Martinez (Stanford)

Daniel Gargas (LBL)  
Filip Furche (Irvine)  
Artem Masunov (UCF)

Koen Binnemans (KU Leuven, Belgium)  
Markus Haase (U. Osnabrück)

**Organizers:** Dmitri Kilin ([Dmitri.Kilin@usd.edu](mailto:Dmitri.Kilin@usd.edu), USD), Svetlana Kilina (NDSU)

**Registration:** <http://www.telluridescience.org/meetings/current>



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